

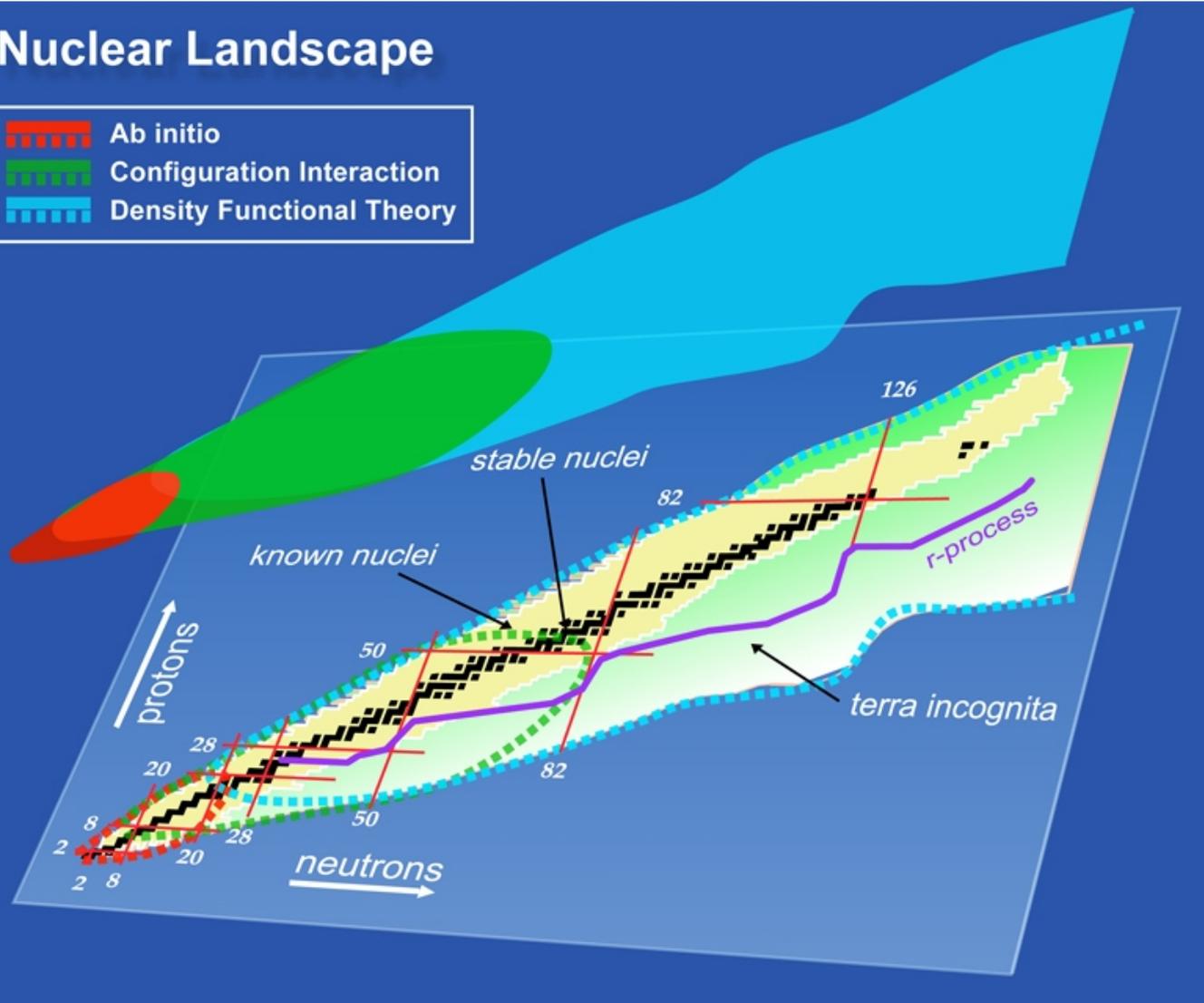
# The Nuclear Many-Body Problem

## Lecture 3

- Shell structure in nuclei and the phenomenological shell model approach to nuclear structure
- Ab-initio approach to nuclear structure. Green's function Monte-Carlo and No-Core Shell-Model.

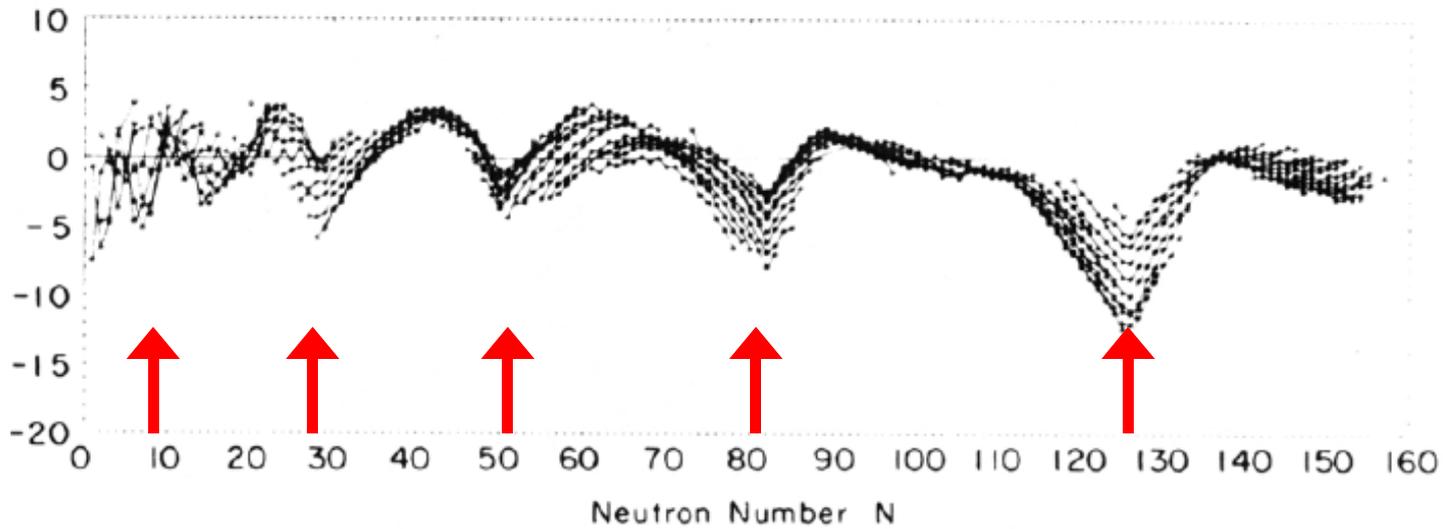
# Roadmap for Theory of Nuclei

## Nuclear Landscape



Main goal : To arrive at a comprehensive description of all nuclei and low-energy reactions from the basic interactions between the constituent nucleons

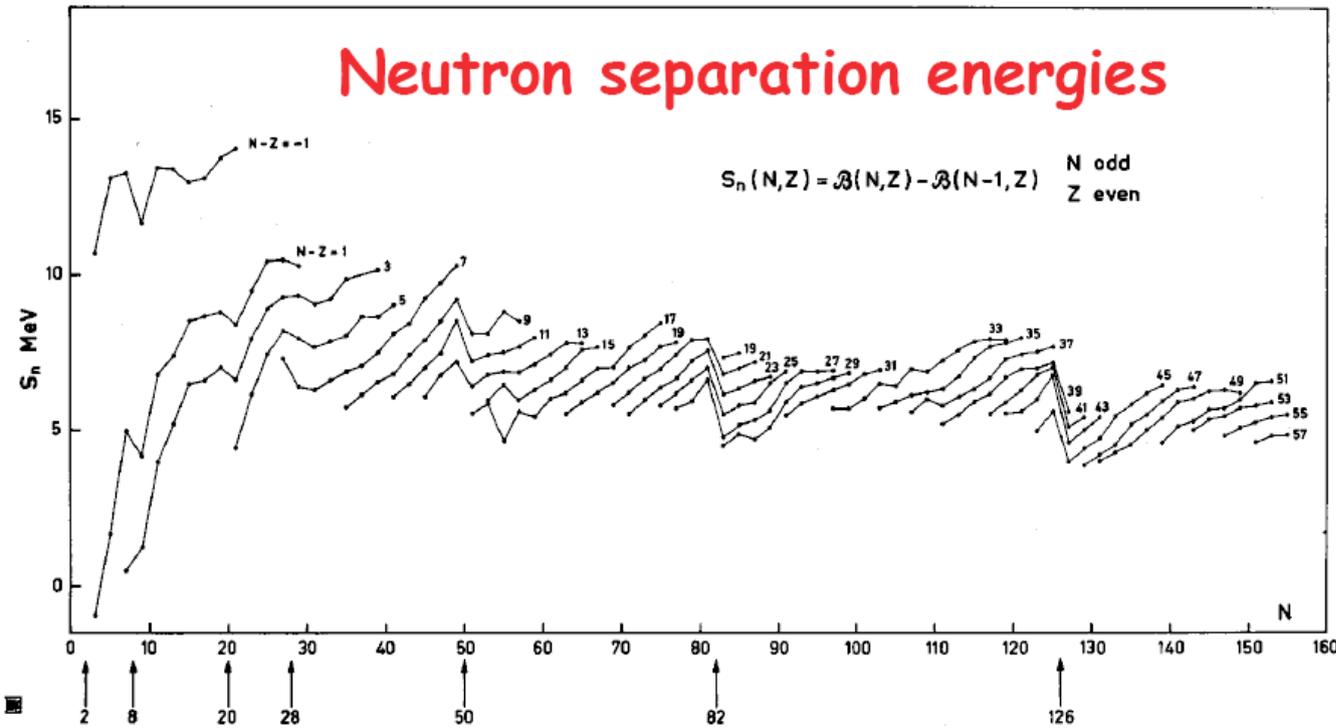
# Shell structure in nuclei



From W.D. Meyers and W.J. Swiatecki, Nucl. Phys. **81**, 1 (1966).

Mass differences: Liquid drop – experiment. Minima at closed shells.

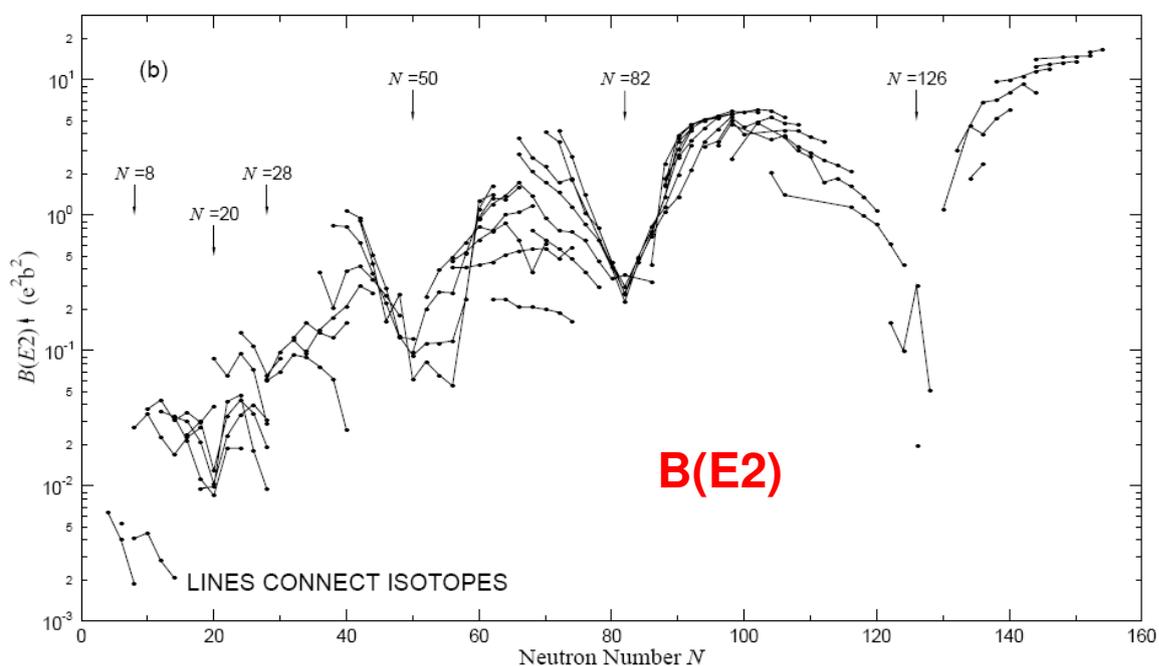
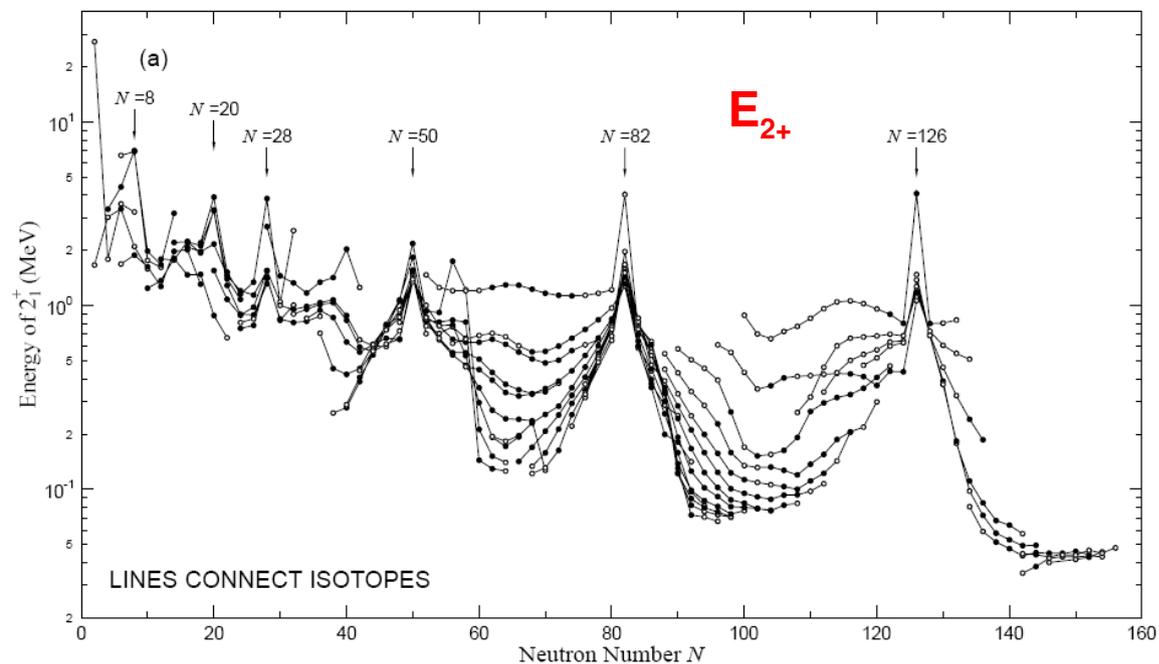
## Neutron separation energies



Relatively expensive to remove a neutron from a closed neutron shell.

Bohr & Mottelson, Nuclear Structure.

# Shell structure cont'd



Nuclei with magic  $N$

- Relatively high-lying first  $2^+$  excited state
- Relatively low  $B(E2)$  transition strength

# 1963 Nobel Prize in Physics



Maria Goeppert-Mayer



J. Hans D. Jensen

“for their discoveries concerning nuclear shell structure”

# Magic numbers

$$H_0 = \sum_{i=1}^A \left( \frac{\hbar^2}{2M} \nabla^2 + \frac{m}{2} \omega^2 r^2 \right)$$

$$E = \hbar\omega(2n+1-1/2)$$

$$\varphi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\vartheta, \varphi)$$

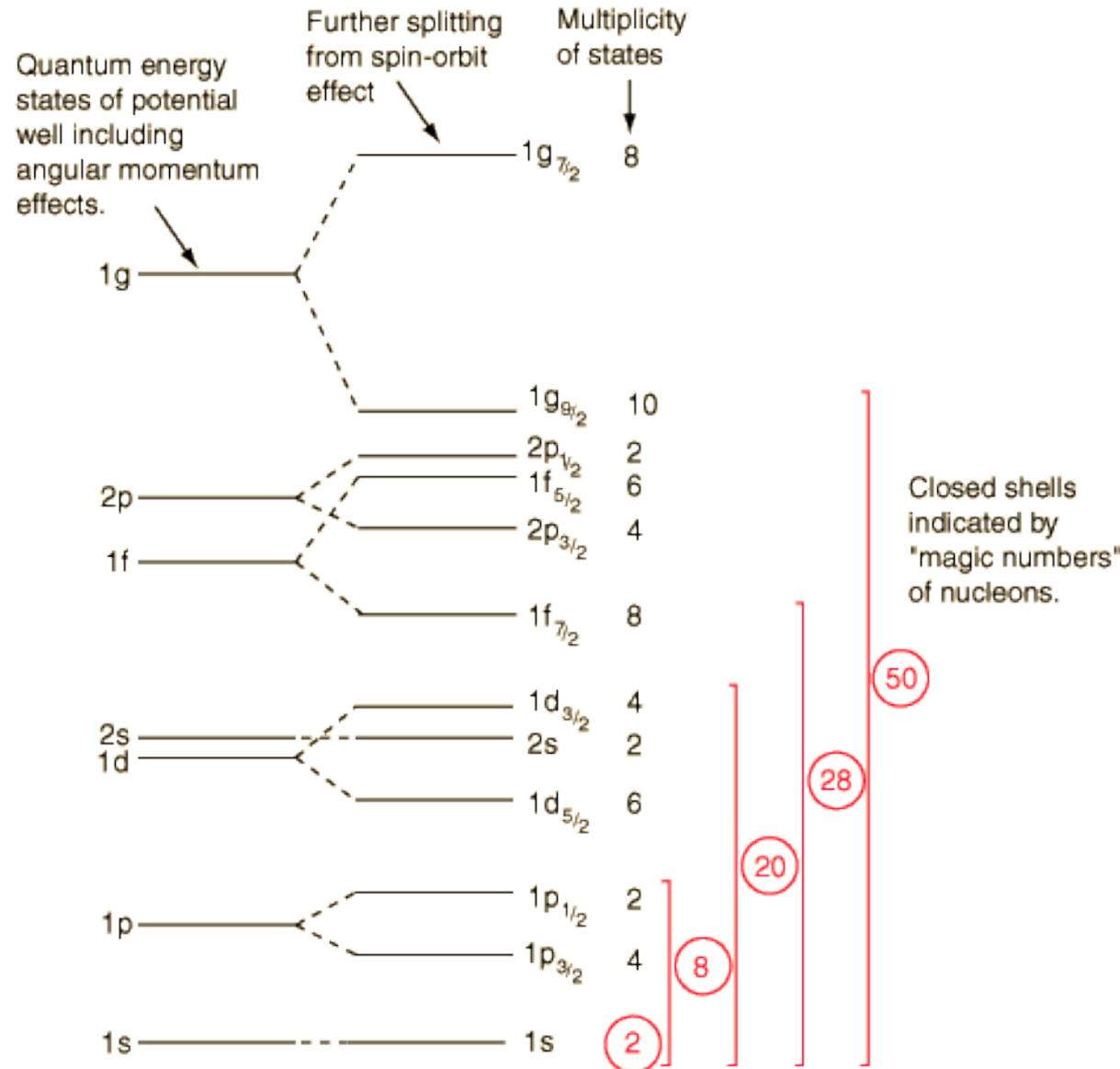
$$R_{nl}(r) \sim r^l e^{-r^2} \times [\text{hypergeometric function in } r^2]$$

$$\varphi_{nljz}(\vec{r}) = R_{nl}(r) [Y_l(\hat{r}) \otimes \chi_{\frac{1}{2}}^S]^{jj_z}$$

$$[Y_l(\hat{r}) \otimes \chi_{\frac{1}{2}}^S]^{jj_z} = \sum_{ms_z} (lm \frac{1}{2} s_z | jj_z) Y_{lm}(\hat{r}) \chi_{\frac{1}{2} s_z}^S$$

$$|\phi_\alpha\rangle = |nljmt_z\rangle \quad j = l + 1/2$$

Need spin-orbit force to explain magic numbers beyond 20.



$$H_{SM} = \sum_{i=1}^A \left( \frac{\hbar^2}{2M} \nabla^2 + \frac{m}{2} \omega^2 r^2 + \eta_l \vec{l}^2 + \xi_{ls} \vec{l} \cdot \vec{s} \right)$$

# Does shell structure change in neutron rich nuclei ?

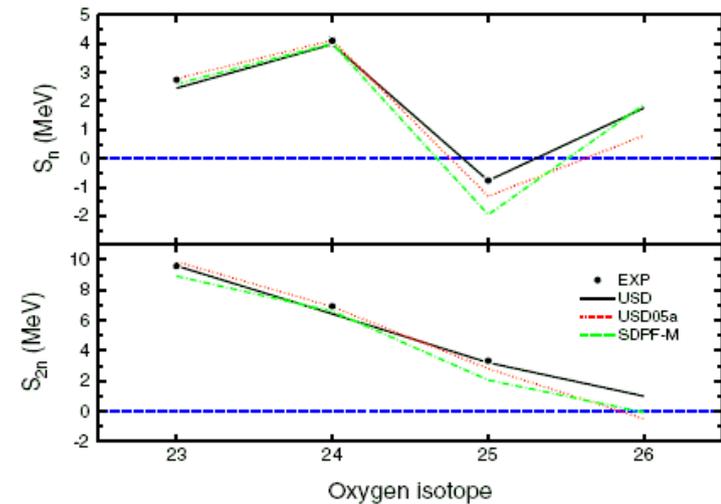
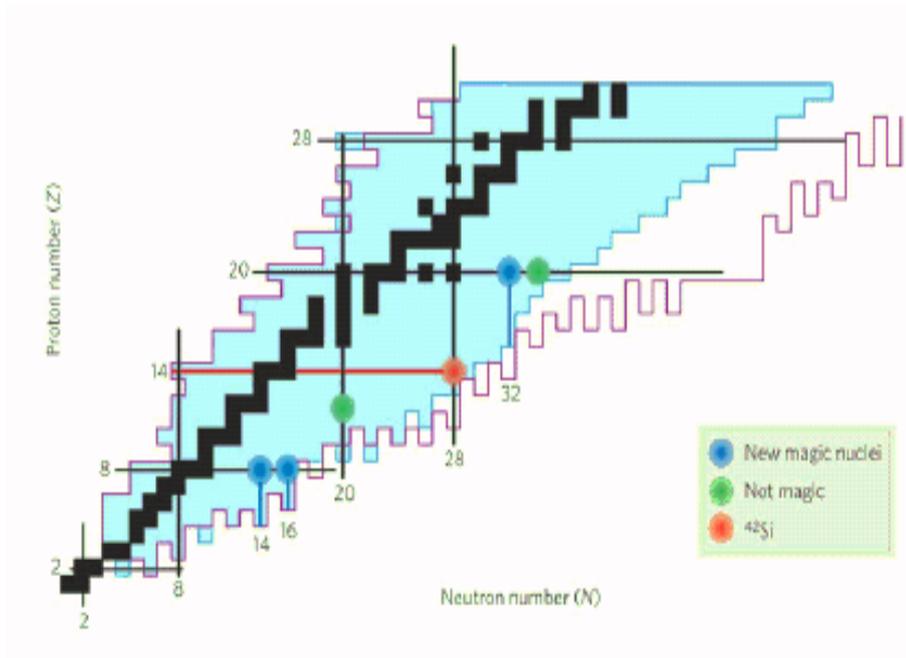


FIG. 4 (color online). The experimental [25,26] (data points) and theoretical [13–15] (lines) one- and two-neutron separation energies for the  $N = 15$ – $18$  oxygen isotopes. The experimental error is shown if it is larger than the symbol size.

Answer: Yes Indeed! Magic numbers fluctuate when one moves away from stability !!!

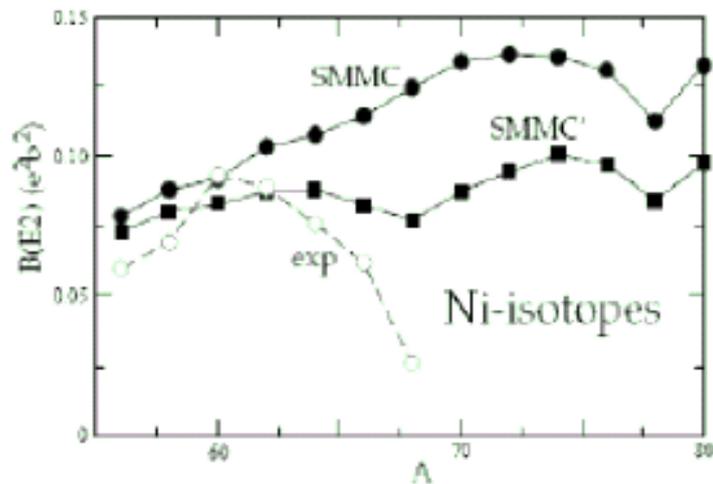
C.R. Hoffman PRL, 100, 152502 (2008)  
Fridmann et al. Nature 435, 922 (2005)  
(comment) Jansens, Nature 435, 207(2005)

# How magic is the magic nucleus $68\text{Ni}$ ?

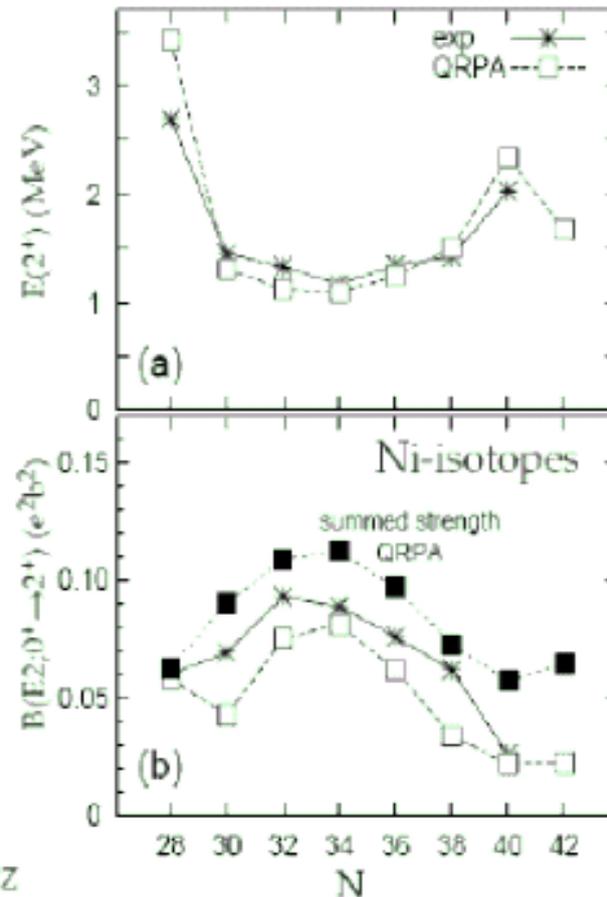
- low-lying  $0^+_2$  level
- higher energy of the  $2^+_1$
- small value of  $B(E2, 0^+_1 \rightarrow 2^+_1)$



interpreted as evidence for magicity!



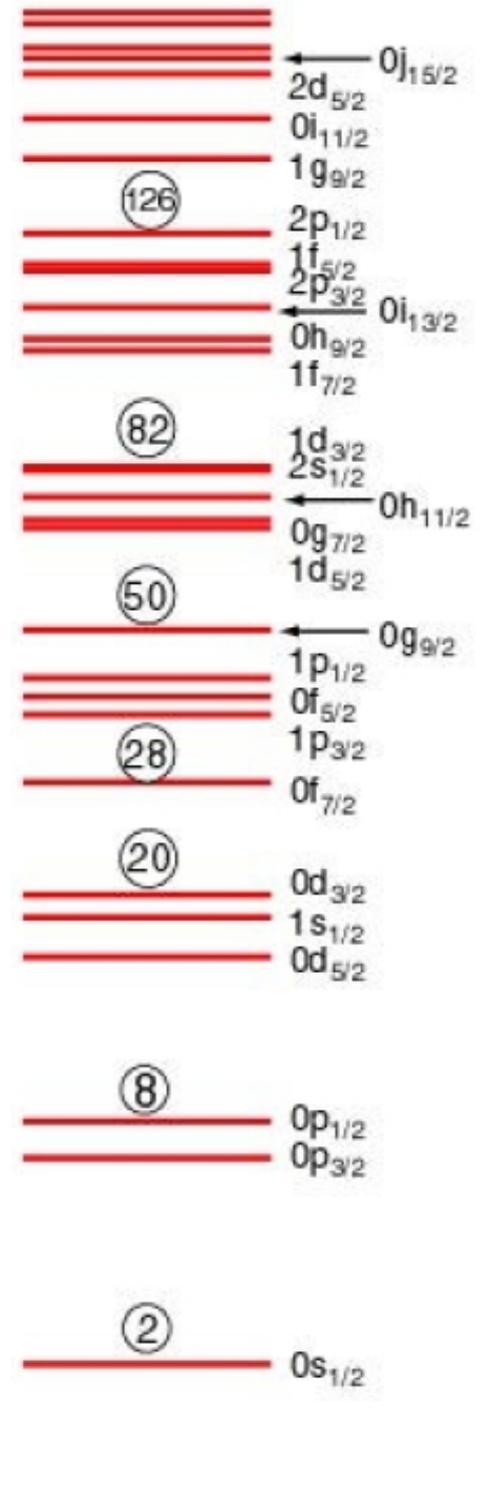
Shell-model Monte-Carlo total summed  $B(E2)$  strength to the  $2^+$  excited states.



# Traditional shell model

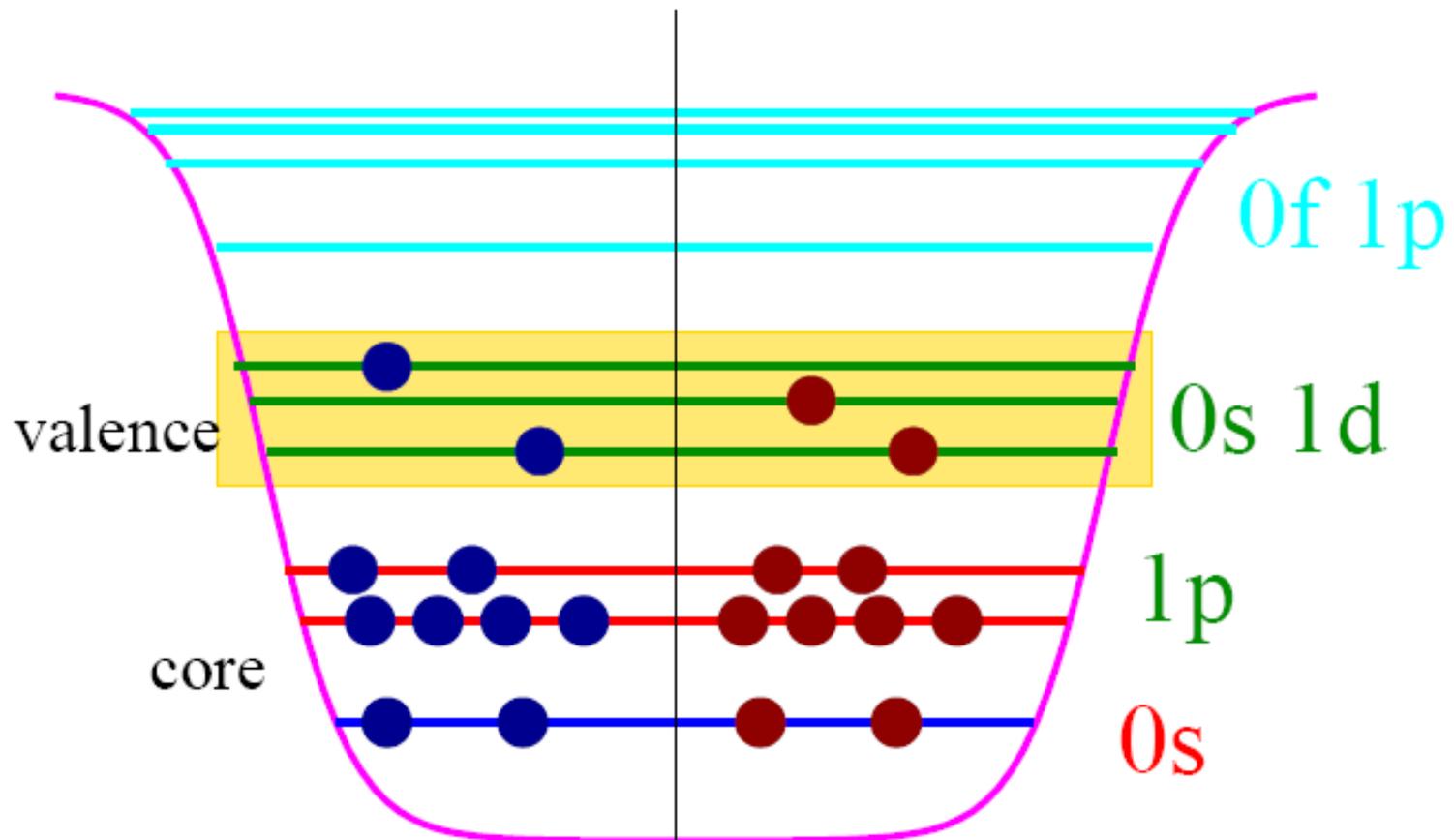
Main idea: Use shell gaps as a truncation of the model space.

- Nucleus  $(N, Z) = \text{Double magic nucleus } (N^*, Z^*) + \text{valence nucleons } (N - N^*, Z - Z^*)$
- Restrict excitation of valence nucleons to one oscillator shell.
  - Problematic: Intruder states and core excitations not contained in model space.
- Examples:
  - pf-shell nuclei:  $^{40}\text{Ca}$  is doubly magic
  - sd-shell nuclei:  $^{16}\text{O}$  is doubly magic
  - p-shell nuclei:  $^4\text{He}$  is doubly magic



# Shell model

Example:  $^{20}\text{Ne}$



# Shell-model Hamiltonian

Hamiltonian governs dynamics of valence nucleons; consists of one-body part and two-body interaction:

$$\hat{H} = \sum_j \varepsilon_j \hat{a}_j^\dagger \hat{a}_j + \sum_{JT j_1 j_2 j'_1 j'_2} \langle j_1 j_2 | \hat{V} | j'_1 j'_2 \rangle_{JT} \hat{A}_{JT; j_1 j_2}^\dagger \hat{A}_{JT; j'_1 j'_2}$$

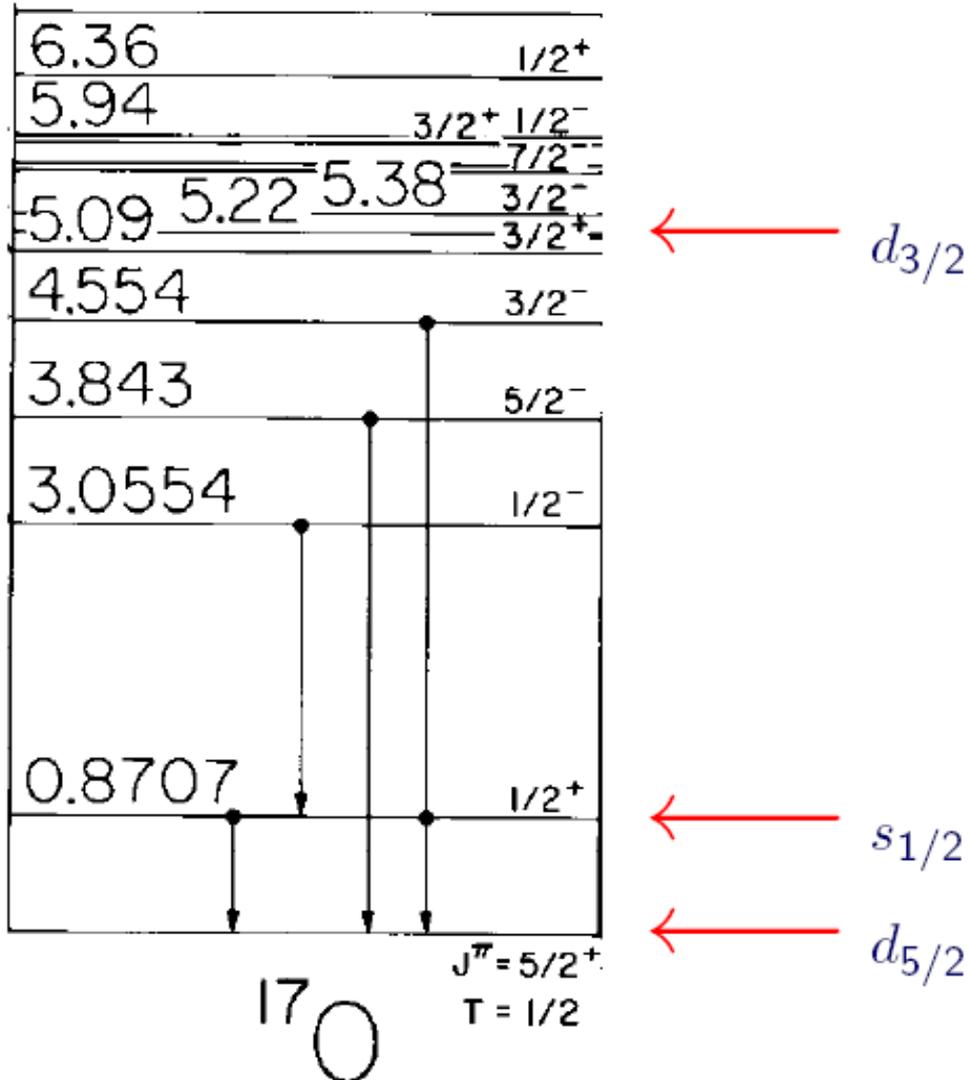
Single-particle energies  
(SPE)

Two-body matrix elements (TBME)  
coupled to good spin and isospin

Annihilates pair of fermions

**Q:** How does one determine the SPE and the TBME?

# Empirical determination of SPE and TBME



- Determine SPE from neighbors of closed shell nuclei having mass  
 $A = \text{closed core} + 1$
- Determine TBME from nuclei with mass  
 $A = \text{closed core} + 2$ .
- The results of such Hamiltonians become inaccurate for nuclei with a larger number of valence nucleons.
- **Thus: More theory needed.**

# Effective shell-model interaction: G-matrix

- Start from a microscopic high-precision two-body potential
- Include in-medium effects in G-matrix
- Bethe-Goldstone equation

$$G = V + V \frac{Q_P}{E - H_0} G$$

microscopic bare interaction  $\rightarrow$   $V$

$\rightarrow$   $Q_P$  Pauli operator blocks occupied states (core)

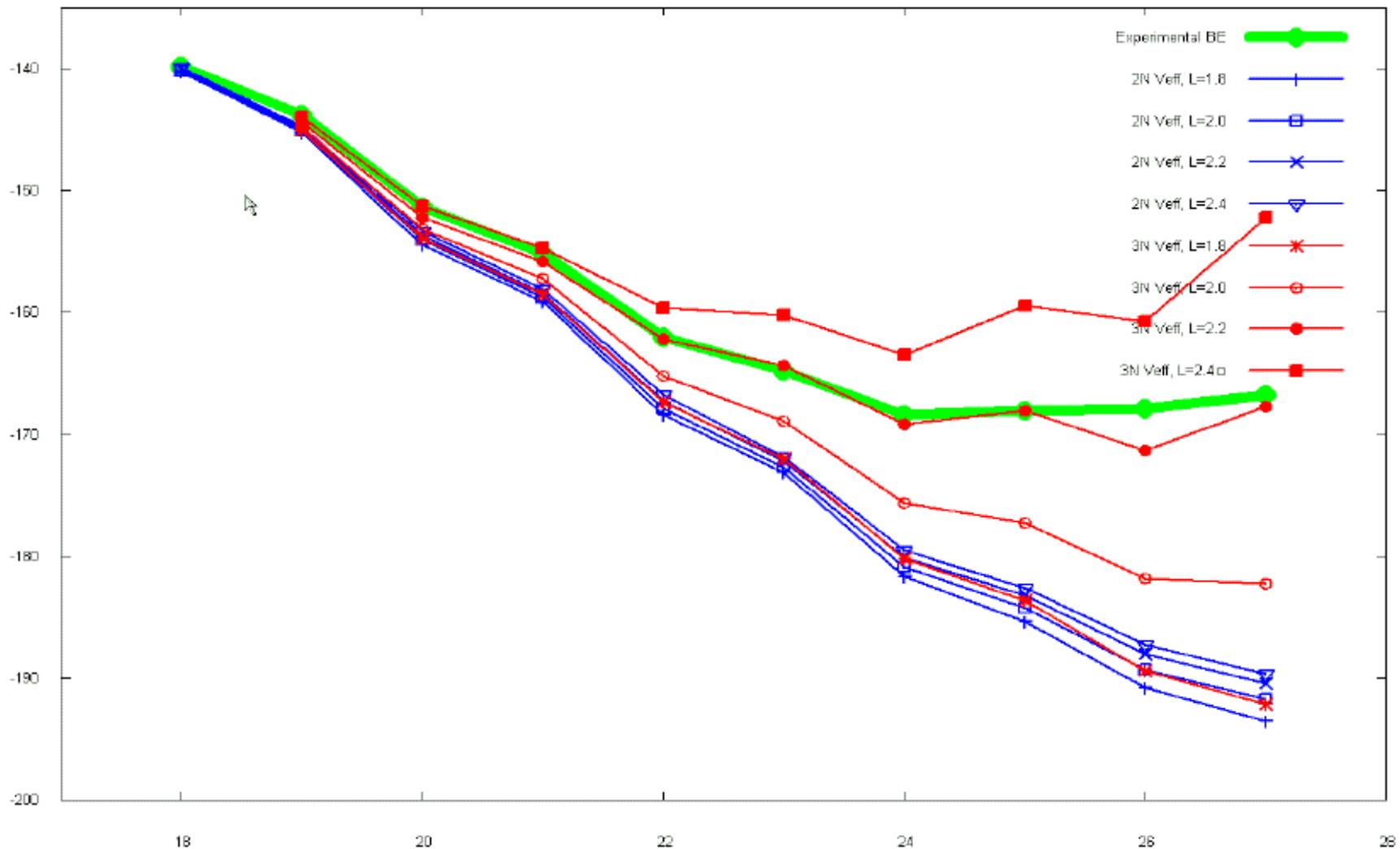
$\uparrow$   $H_0$  Single-particle Hamiltonian

- Formal solution:

$$G = \frac{V}{1 - V Q_P / (E - H_0)}$$

- Properties: in-medium effects renormalize hard core.

# Shell model calculations of Oxygen isotopes using v-lowk and effective 2- and 3-body forces.



From Maxim Kartamyshev

# Shell-model results for neutron-rich pf-shell nuclei.

Subshell closure at neutron number  $N=32$  in neutron rich pf-shell nuclei (enhanced energy of excited  $2^+$  state).

No new  $N=34$  subshell.

S. N. Liddick et al, PRL 92 (2004) 072502.

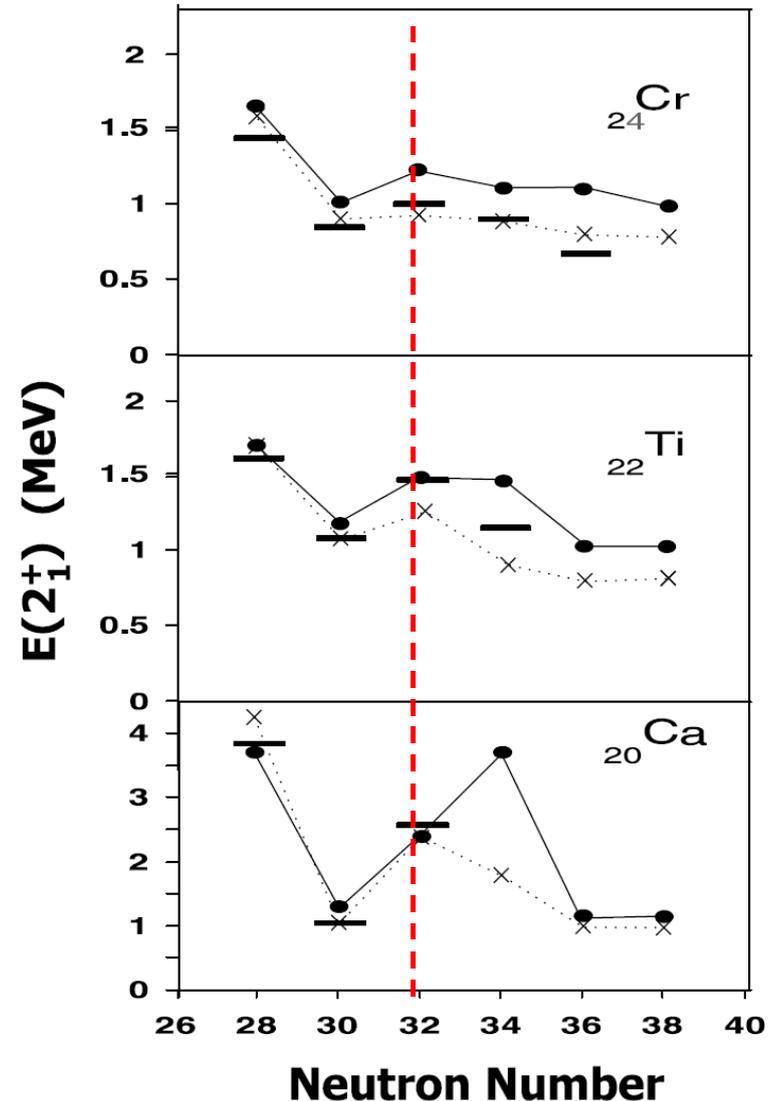


FIG. 3.  $E(2_1^+)$  values versus neutron number for the even-even  $^{24}\text{Cr}$ ,  $^{22}\text{Ti}$ , and  $^{20}\text{Ca}$  isotopes. Experimental values are denoted by dashes. Shell model calculations using the GXPF1 [14] and KB3G [22] interactions are shown as filled circles and crosses, respectively.

# Solving the ab-initio quantum many-body problem

Exact or virtually exact solutions available for:

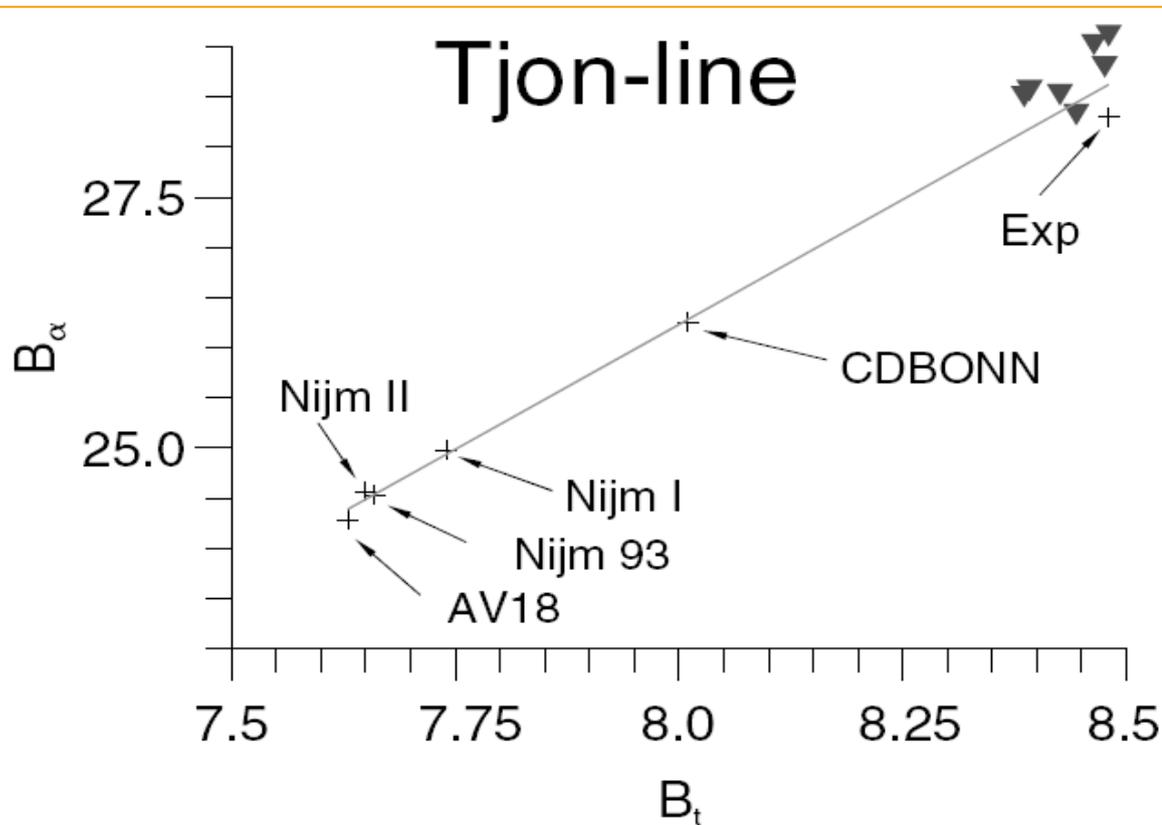
- $A=3$ : solution of Faddeev equation.
- $A=4$ : solvable via Faddeev-Yakubowski approach.
- Light nuclei (up to  $A=12$  at present): Green's function Monte Carlo (GFMC); virtually exact; limited to certain forms of interactions.

Highly accurate approximate solutions available for:

- Light nuclei (up to  $A=16$  at present): No-core Shell model (NCSM); truncation in model space.
- Light and medium mass region ( $A=4, 16, 40$  at present): Coupled cluster theory; truncation in model space and correlations.

# 1990s: High precision NN potential models

- Phenomenological models based on meson exchange.
- Contain about 40 parameters; determined by fit to phase shifts/deuteron.
- Reproduce NN phase shifts with a  $\chi^2/\text{datum}$  very close to 1.0.
- “Nearly perfect” two-body physics.



Different two-body potential models disagree on structure of triton and alpha particle.

With additional **three-nucleon forces**, agreement with experiment is possible.

(Three-nucleon force differs for different two-body potentials.)

Four-body forces very small.

# Green's Function Monte Carlo

Idea:

2. Determine accurate approximate wave function via variation of the energy (The high-dimensional integrals are done via Monte Carlo integration).

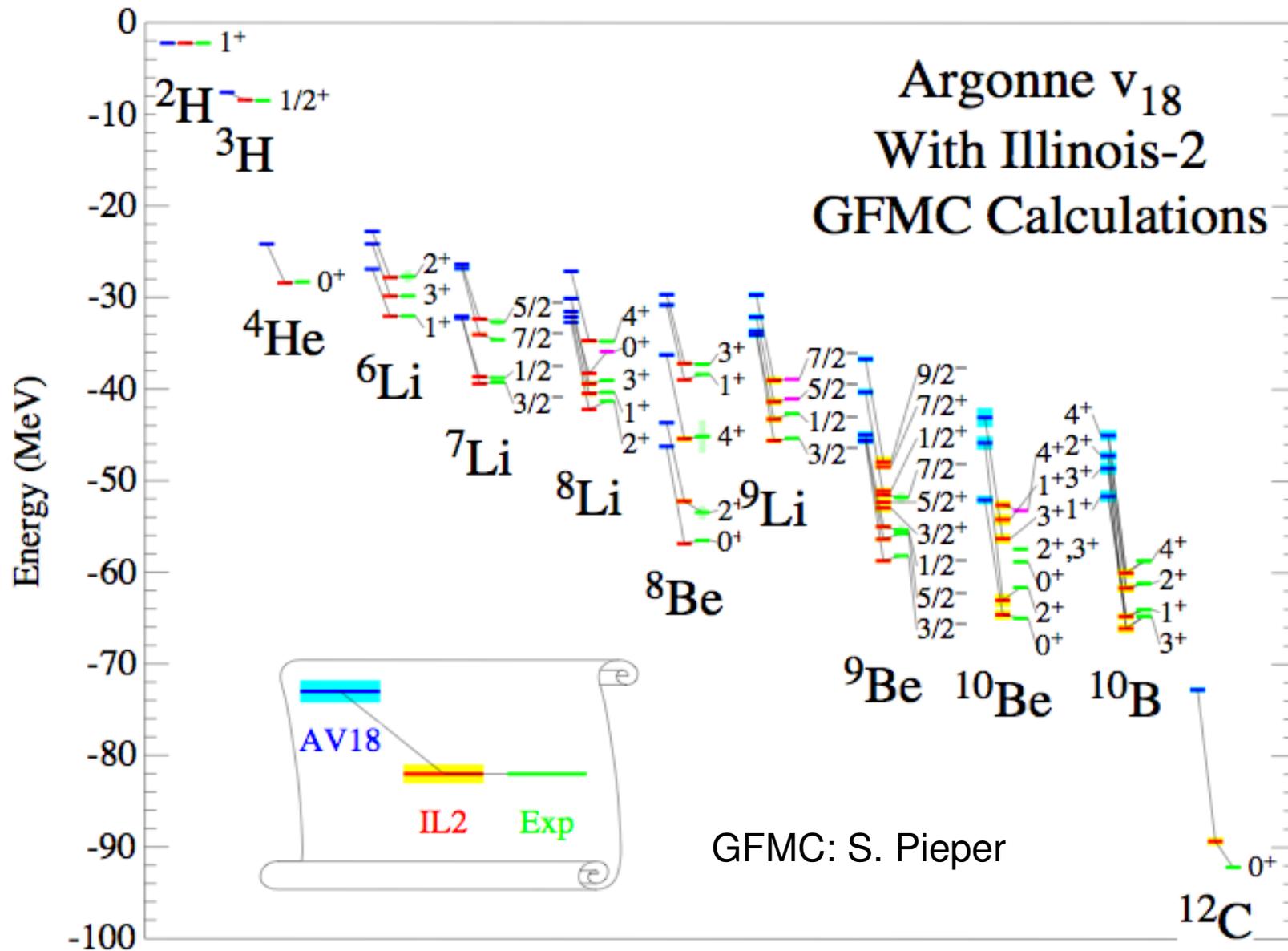
$$E = \frac{\langle \Psi_{\text{trial}} | \hat{H} | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle}$$

6. Refine wave function and energy via projection with Green's function

$$|\Psi\rangle = \lim_{\tau \rightarrow \infty} e^{-\tau(\hat{H}-E)} |\Psi_{\text{trial}}\rangle$$

- ☺ Virtually exact method.
- ☹ Limited to certain forms of Hamiltonians; computationally expensive method.

# GFMC results for light nuclei



1-2% calculations of  $A = 6 - 12$  nuclear energies are possible  
excited states with the same quantum numbers computed

# GFMC calculations of $n$ - $\alpha$ scattering

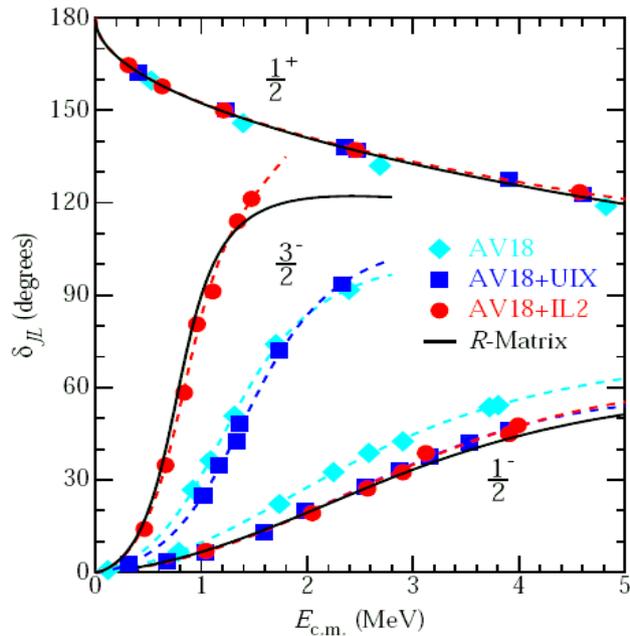


FIG. 1: (Color online) Phase shifts for  $n$ - $\alpha$  scattering. Filled symbols (with statistical errors smaller than the symbols) are GFMC results; dashed curves are fits described in the text; and solid curves are from an  $R$ -matrix fit to data [14].

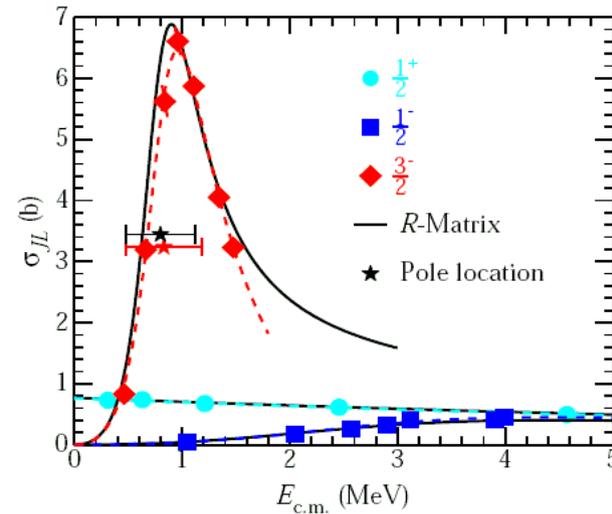


FIG. 2: (Color online) Calculated and  $R$ -matrix partial-wave cross sections. The calculations, shown with their Monte Carlo error bars, are for the AV18+IL2 Hamiltonian. Stars show the pole energies in  $3/2^-$  scattering for the  $R$ -matrix fit and for AV18+IL2, with the bars indicating the imaginary part.

p3/2 resonance :  $0.83 - 0.35i$  (exp  $0.798 - 0.324i$ )  
 p1/2 resonance :  $2.07 - 2.6i$  (exp  $2.07 - 2.79i$ )

K. Nellott et al, Phys. Rev. Lett 99, 022502 ( 2007 )

# No core shell model

Idea: Solve the A-body problem in a harmonic oscillator basis.

2. Take K single particle orbitals
3. Construct a basis of Slater determinants
4. Express Hamiltonian in this basis
5. Find low-lying states via diagonalization

☺ Get eigenstates and energies

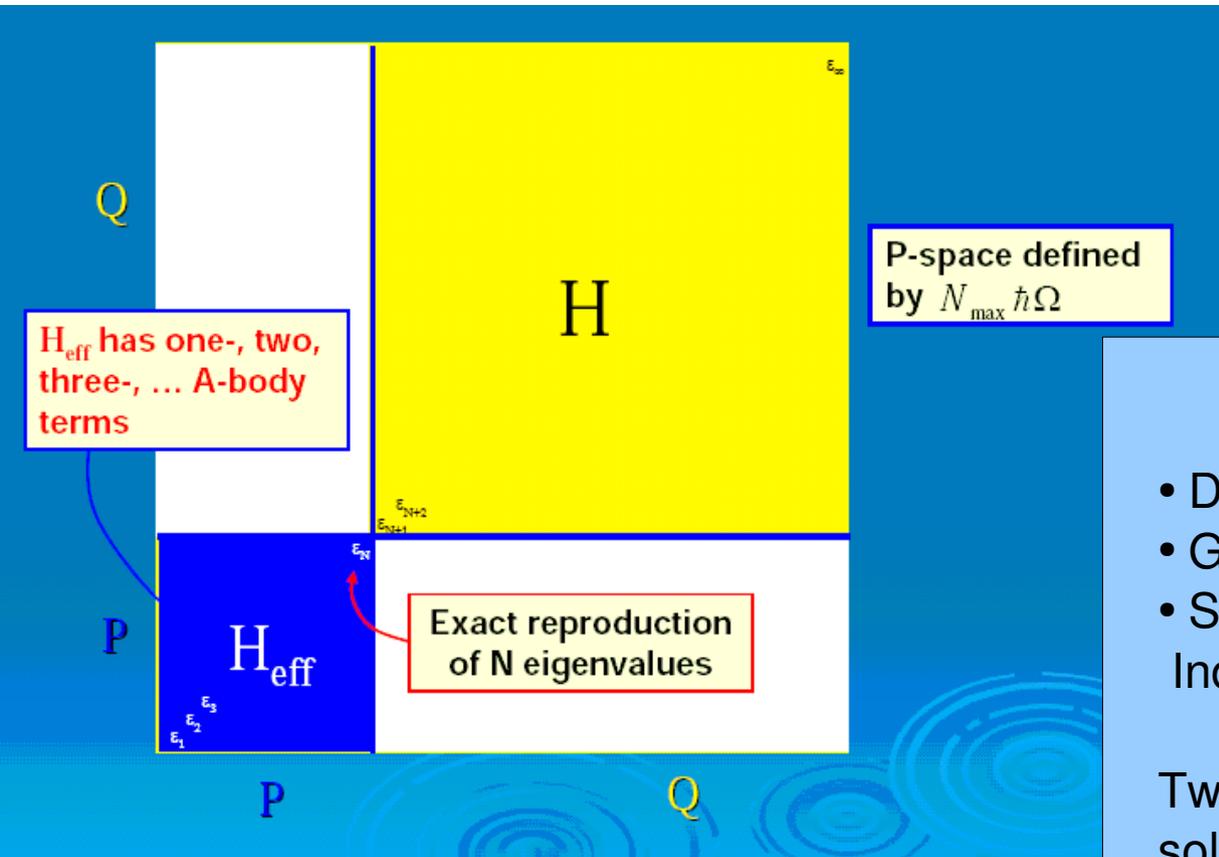
☺ No restrictions regarding Hamiltonian

☹ Number of configurations and resulting matrix very large: There are

$$\binom{K}{A} = \frac{K!}{(K-A)!A!}$$

ways to distribute A nucleons over K single-particle orbitals.

# The general idea behind effective interactions and the Lee-Suzuki similarity transformation.



- Define a model space  $P$
- Generate an effective interaction in  $P$
- Solve the many-body problem  
Induces many-body forces

Two ways of converging to the bare solution :

1. Increase model space  $P$  until convergence
2. Include induced many-body forces, reproduces bare solution

# Working in a finite model space

NCSM and Coupled-cluster theory solve the Schroedinger equation in a model space with a *finite* (albeit large) number of configurations or basis states.

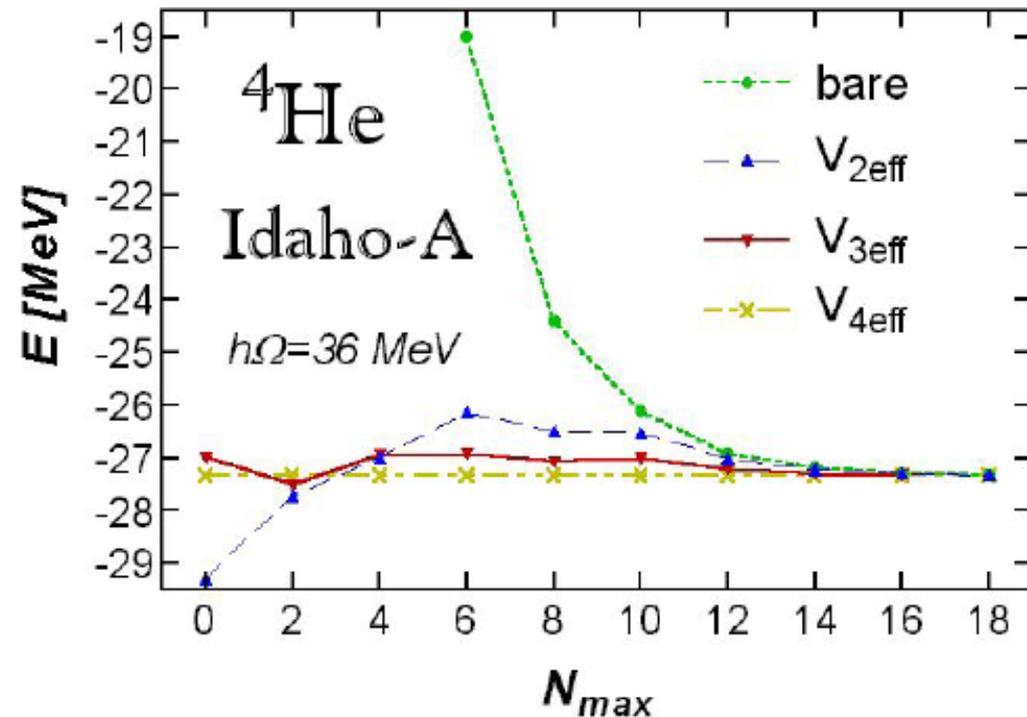
Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

**Solution:** Get rid of the high-momentum modes via a renormalization procedure. (Vlow-k is an example)

## Price tag:

Generation of 3, 4, ..., A-body forces unavoidable.

Observables other than the energy also need to be transformed.



E. Ormand

<http://www.phy.ornl.gov/npss03/ormand2.ppt>

# Theorists agree with each other

PHYSICAL REVIEW C, VOLUME 64, 044001

## Benchmark test calculation of a four-nucleon bound state

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(Received 20 April 2001; published 27 August 2001)

In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this

***VN interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.***

TABLE I. The expectation values  $\langle T \rangle$  and  $\langle V \rangle$  of kinetic and potential energies, the binding energies  $E_b$  in MeV, and the radius in fm.

Method	$\langle T \rangle$	$\langle V \rangle$	$E_b$	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	-128.33(10)	-25.94(5)	1.485(3)
CRCGV	102.30	-128.20	-25.90	1.482
SVM	102.35	-128.27	-25.92	1.486
HH	102.44	-128.34	-25.90(1)	1.483
GFMC	102.3(1.0)	-128.25(1.0)	-25.93(2)	1.490(5)
NCSM	103.35	-129.45	-25.80(20)	1.485
EIHH	100.8(9)	-126.7(9)	-25.944(10)	1.486

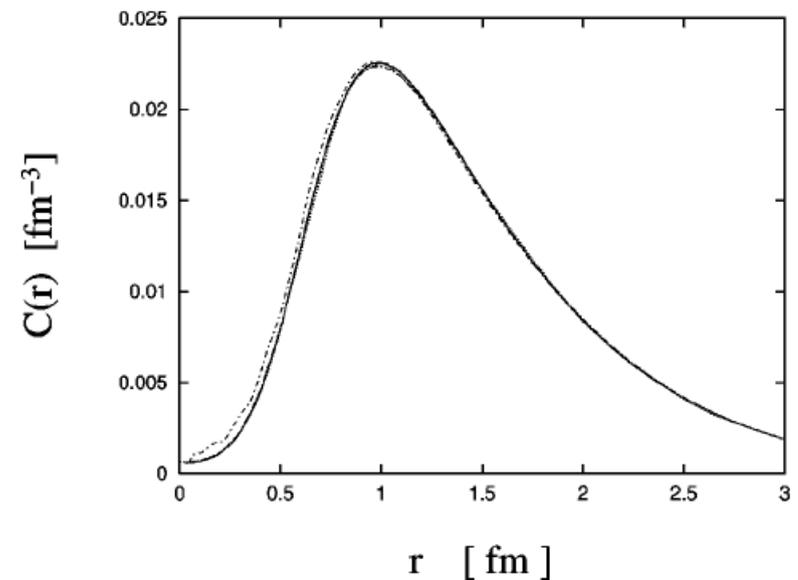
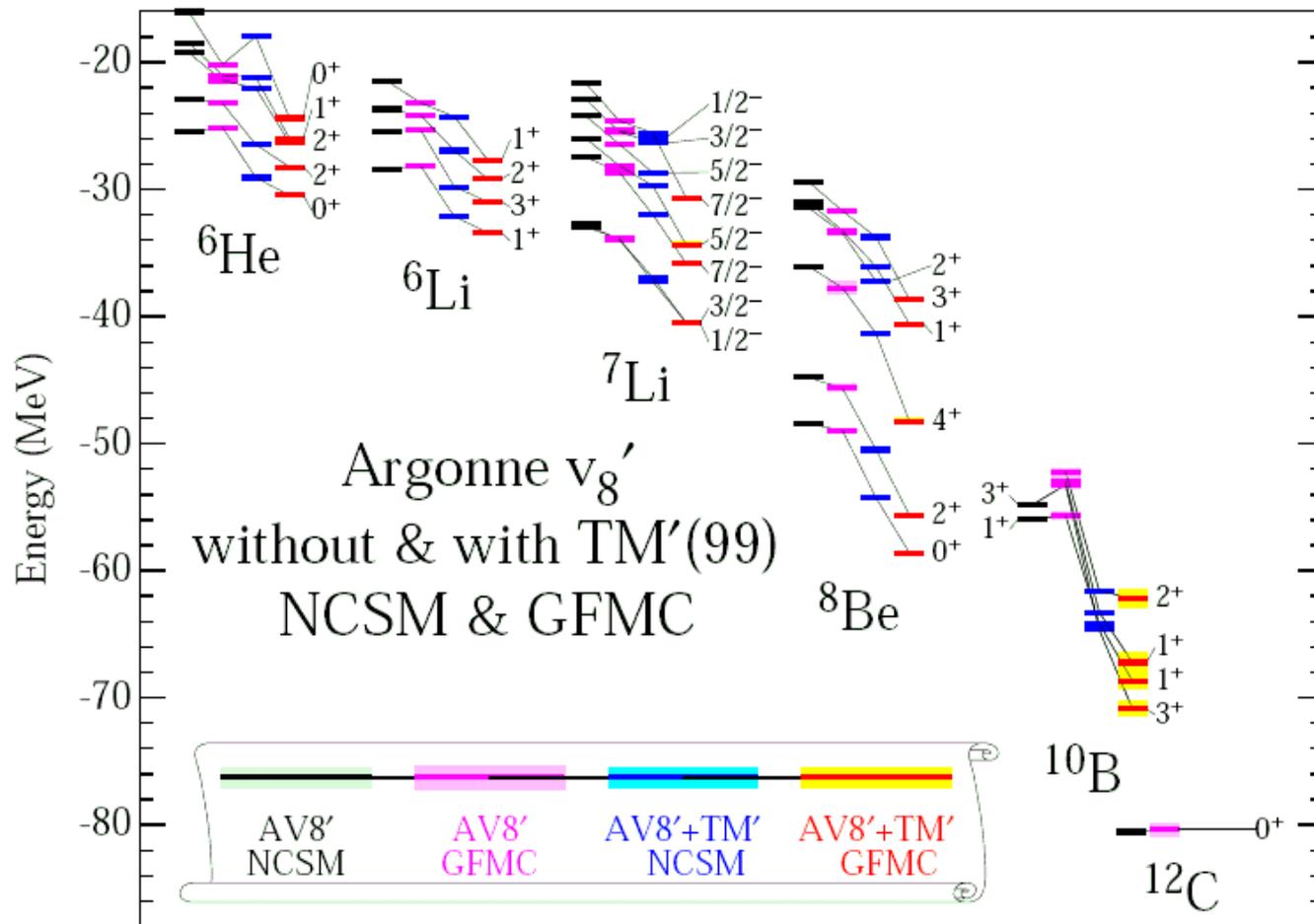


FIG. 1. Correlation functions in the different calculational schemes: EIHH (dashed-dotted curves), FY, CRCGV, SVM, HH, and NCSM (overlapping curves).

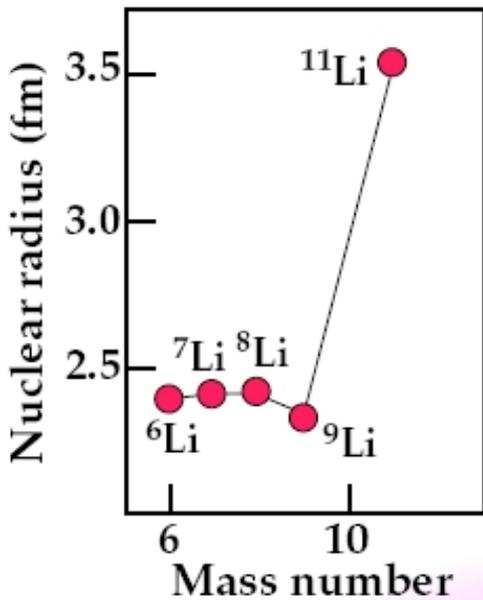
# Comparison between NCSM and GFMC



S. Pieper Nucl. Phys. A  
751 (2005) 516-532

Figure 6. Comparison of NCSM and GFMC energies for the AV8' and AV8'+TM' Hamiltonians.

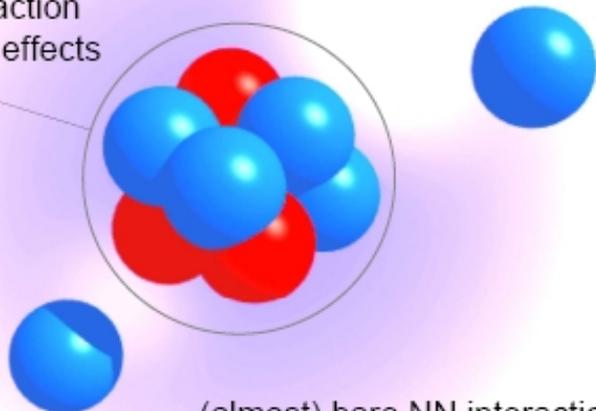
# Ab-initio calculations of charge radii of Li isotopes



I. Tanihata et al.  
Phys. Rev. Lett. 55, 2676 (1985)

Interaction cross section  
measurements at Bevalac  
(790 MeV/u)

effective NN interaction  
strong in-medium effects



(almost) bare NN interaction  
weak in-medium effects

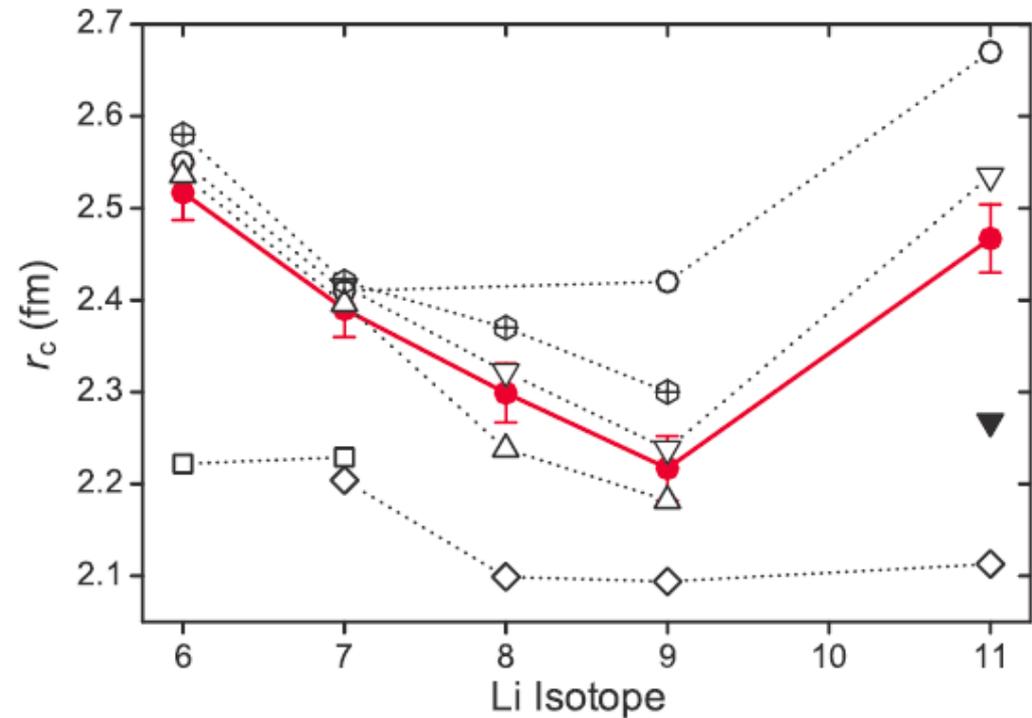
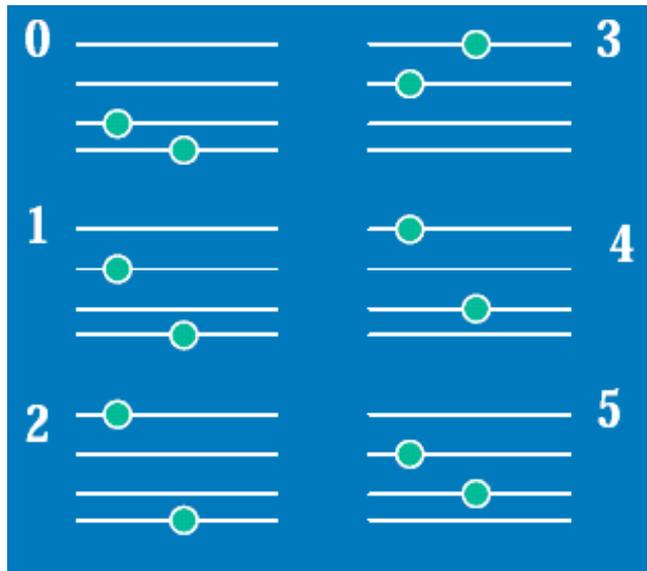


FIG. 2 (color online). Experimental charge radii of lithium isotopes (red,  $\bullet$ ) compared with theoretical predictions:  $\Delta$ : GFMC calculations [4,22],  $\nabla$ : SVMC model [27,28] ( $\blacktriangledown$ : assuming a frozen  ${}^9\text{Li}$  core),  $\oplus$ : FMD [26],  $\circ$ : DCM [19],  $\square$  and  $\diamond$ : *ab initio* NCSM [23,24].

R. Sanchez et al, PRL 96 (2006) 33002.

# The $N!$ catastrophe.

## Specific example: 2 particles in 4 states



$$I = 0 \quad a_2^+ a_1^+ |--\rangle = |1100\rangle = |\Phi_0\rangle$$

$$I = 1 \quad a_3^+ a_1^+ |--\rangle = |1010\rangle = |\Phi_1\rangle$$

$$I = 2 \quad a_4^+ a_1^+ |--\rangle = |1001\rangle = |\Phi_2\rangle$$

$$I = 3 \quad a_3^+ a_2^+ |--\rangle = |0110\rangle = |\Phi_3\rangle$$

$$I = 4 \quad a_4^+ a_2^+ |--\rangle = |0101\rangle = |\Phi_4\rangle$$

$$I = 5 \quad a_4^+ a_3^+ |--\rangle = |0011\rangle = |\Phi_5\rangle$$

Scaling: Number of basis states

Oops.. These are huge numbers

Problem : How to deal with such large dimensions

$n$  = number of particles;

$N$  = number of single - particle states

$$C(N, n) = \frac{N!}{(N-n)! n!}$$

$$C(10, 100) = 1.7 \times 10^{13}$$

$$C(1000, 100) = 6 \times 10^{139}$$

# Summary

- Shell model a powerful tool for understanding of nuclear structure.
- Shell model calculations based on microscopic interactions
  - Adjustments are needed
  - Due to neglected three body forces (?!)
- Effective interactions have reached maturity to make predictions, and to help understanding experimental data
- Green's function Monte-Carlo and No-core Shell-model capable of ab-initio description of nuclei with  $A < 12$
- Due to factorial scaling of the method, very difficult to extend to heavier systems.
- Need accurate method with softer scaling in order to extend the ab-initio program to heavier systems.